

Quantum phase transition and critical phenomena

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Abstract . We intend to describe briefly the generic features associated with the zero-temperature transition in quantum mechanical systems. We elucidate the discussion of the introductory section using the very common example of Ising model in a transverse field. We discuss the method of fermionisation for one dimensional systems. The quantum-classical correspondence is discussed using Suzuki-Trotter method. We then introduce the quantum rotor model and discuss its spherical limit. We finally discuss novel features arising due to the presence of quenched randomness in the quantum Ising and rotor systems.

Keywords Quantum phase transitions, Quantum Ising models, Quantum rotor models

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1. Introduction

1.1 Introduction to classical phase transitions :

Let us consider a many-body system, like a magnet, consisting of many internal degrees of freedom (here the spins). If the degrees of freedom themselves interact in a cooperative interaction, then at sufficiently low temperature the entire thermodynamic system shows some macroscopic (long-range) order, *e.g.*, net spontaneous magnetisation in a ferromagnet may attain a non-zero value at low temperature due to the ferromagnetic interaction between the spins. As the temperature (thermal noise) increases, the thermal fluctuations allow for costly (spin) configurations which have higher energies (E), through the Boltzman probability distribution ($\exp(-E/k_B T)$), where k_B is the Boltzman constant. This thermal fluctuations introduce disorder at any finite temperature, and the order is destroyed ; spontaneous magnetisation starts decreasing with increasing temperature. Finally at a well defined temperature, called the transition temperature T_c , the macroscopic order m disappears, the ferromagnet (for $T < T_c$) becomes paramagnet (for $T > T_c$). The observable, usually unique, changing from non-zero to the zero value (in ferromagnets, the spontaneous magnetisation) in a phase transition is called the order parameter.

One may represent the thermodynamic state of such systems by the equation of state: say $m = m(T, h)$, where T, h etc. denotes temperature, magnetic field etc. As discussed in the last

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paragraph, this equation of state changes drastically (from $m \neq 0$ to $m = 0$) at the transition point. Similar is the case for a fluid, or other systems undergoing phase transition. Usually in thermodynamics, we define some "potentials", called the free energy F ($= E - TS$, for the Helmholtz' free energy ; E denotes internal energy of the system and S denotes the entropy of the system), such that the various thermodynamic parameters can be obtained as various derivatives of the free energy ; e.g., order parameter m , entropy S specific heat C and susceptibility χ go as

$$m \sim \frac{\partial F}{\partial h} ; S \sim \frac{\partial F}{\partial T} ; C = \frac{\partial S}{\partial T} \sim \frac{\partial^2 F}{\partial T^2} ; \chi \sim \frac{\partial m}{\partial h} \sim \frac{\partial^2 F}{\partial h^2}$$

respectively. Since, across any phase transition point (or surface), the equation of state of the thermodynamic system changes abruptly, one can define an order of transition by noting which order of the derivative of the free energy changes discontinuously there ; e.g., if the magnetisation m changes continuously from nonzero value to the zero value at T_c , but the susceptibility χ and the specific heat C discontinuously changes or diverges at T_c , we call the transition a second order one. In case of ice melting to water, a latent heat ($= T \Delta S$) appears due to a discontinuous change (ΔS) in the entropy. Similar changes also occur in volume ($v = \partial F / \partial p$), where p denotes the pressure. Thus such transitions are first order transition.

It has been observed that the transition point (here, say the transition temperature T_c in the example of the ferromagnet) depends on many details of the system ; the interaction strength within the basic degrees of freedom, crystal structure etc. However, careful observations revealed that the variations in the thermodynamic properties of various systems undergoing second order phase transitions (having widely different transition temperature e.g., $T_c = 4.2^\circ K$ for superfluid helium to a large class of isotropic (XY-like) magnets having $T_c = 500^\circ K$ have remarkably identical behaviour. This is called the "Universality". In order to be more precise, let us define exponents : if we express the variation of any thermodynamic quantity Q (which can be related to some appropriate derivative of the free energy F) near T_c as

$$Q \sim \text{const} + |T - T_c|^{-\alpha}$$

with the exponent α (which can take +ve or -ve values), then we find that α does not depend on the details of the system at all ! For example, observing the specific heat and magnetisation in magnets of various transition temperature, one finds that when they are fitted to the form

$$C \sim |T - T_c|^{-\alpha} ; m \sim (T_c - T)^\beta$$

with $\alpha \approx 0.01$ and $\beta \approx 0.33$ for many magnets. One finds [1] that very subtle features of the thermodynamic systems, like the physical dimension of the system, dimension of the degrees of freedom, etc. determines the values of the exponents ; not every details of the systems. The "universality" class of the transition are therefore determined by those subtle features like dimension. It should be clearly stated here, that like the critical temperature the size of the critical region (i.e., the interval of temperature within which the universality is pronounced) is also dependent on the system details.

Another point to be noted is that the exponents are very often nonintegers, indicating that the free energy (after two integration of the sp. heat C , $F - |T - T_c|^{2-\alpha}$ is a singular

function of the thermodynamic variables like temperature etc (since $2 - \alpha$ is also a noninteger, all its derivatives at $T = T_c$ can not exist). It is now believed, that all these singularities come because of a singularity of a basic quantity called the correlation length ξ can be obtained from the average correlation $g(r)$ between two degrees of freedom (say S) at a distance r :

$$g(r) = 0 < (S(0) - \langle S(0) \rangle) (S(r) - \langle S(r) \rangle) \rangle \sim \exp(-r/\xi),$$

where $\langle \dots \rangle$ denotes that average over the thermodynamic ensemble and ξ is the correlation length. $\xi \sim |T - T_c|^{-\nu}$ near the critical point, at the critical point (when ξ diverges) the point correlation function scale as

$$g(r) \sim r^{2+d-\eta}$$

The diverging correlation length is the origin of all singularities arising at the critical point. These two exponents ν and η are two independent exponents which determine other exponents α , β , γ and δ through the following scaling relations. We shall briefly sketch how the *hyperscaling relation* connecting the specific heat exponent α and the correlation length exponent ν is obtained. Let us consider a domain of linear size of the order of the correlation length ξ , so the free energy density should scale as ξ^{-d} , total free energy being constant. On the other hand, near the critical point the free energy density should scale as $|T - T_c|^{2-\alpha} \sim \chi t^{-(2-\alpha)/\nu}$. Comparing these two scaling forms for the free energy density, we obtain the hyperscaling relation

$$2 - \alpha = \nu d.$$

The other scaling relations obtained from similar arguments are the following

$$\begin{aligned}\gamma &= (2 - \eta)\nu, \\ \alpha + 2\beta + \gamma &= 2, \\ \alpha + \beta(1 + \delta) &= 2.\end{aligned}$$

We shall conclude this section with the note that we have here just tried to give a flavour of the beauty and bounty of the subject *classical phase transition*. For detailed and rigorous discussions, we refer to the books cited in the bibliography section. [1-5]

1.2 Introduction to quantum phase transitions :

In the previous section, we have discussed that the most important feature of a second order phase transition is the divergence of correlation length ξ at the finite temperature critical point T_c . The correlation length generally diverges as a power law

$$\xi \sim |T - T_c|^{-\nu}, \quad (1)$$

where as mentioned previously ν is the *universal* critical exponent. So far in our discussion, the effects due to quantum mechanical fluctuations have not been taken into consideration. This is reasonable as we shall discuss later that in finite temperature transitions, thermal fluctuations always dominate over the quantum fluctuations and thus the critical fluctuations are always classical. To see this we recall that in the vicinity of the critical point, not only the spatial correlations become long-range, but the temporal correlation (relaxation time) also diverge at the critical point causing what is known as the "critical slowing down". We here define the classical dynamical exponent z as

$$\tau \sim \xi^z$$

where τ is the relaxation time of the classical model.

We shall now try to see under what conditions the thermal or the quantum fluctuations dominate the physics. Let us compare the thermal energy per degree of freedom, $k_B T$, with the zero point quantum energy per degree of freedom, $\hbar \omega_c$, where ω_c is the frequency of fluctuation. For critical phenomena, the important frequency is the inverse of the relaxation time, i.e., τ^{-1} , which goes to zero at the critical point. Hence, we find

$$\hbar \omega_c \ll k_B T \quad (2)$$

sufficiently close to T_c , even though the underlying Hamiltonian may be quantum mechanical, provided that T_c is finite. More precisely, we need $T - T_c \leq T_c^{1/\nu}$, for the above equation to be valid. Hence as long as T_c is finite, the critical fluctuations will be classical and classical statistical mechanics will suffice to determine the universal critical behaviour.

Let us now consider the situation where we study the phase transitions in a system described by a quantum mechanical Hamiltonian with an additional tunable parameter Δ (apart from temperature), which determines the strength of quantum fluctuations. With the increase of Δ , naturally the quantum fluctuations will be more and thus T_c will be lower. Eventually, at a particular value of $\Delta = \Delta_c$, the critical temperature will vanish! At $T = 0$, there is no thermal fluctuations and hence the transition which occurs varying the control parameter Δ at ($T = 0$) is called the quantum phase transition and the point $T = 0, \Delta = \Delta_c$ is called a quantum critical point. *These transitions take place at absolute zero temperature, when crossing the phase boundary means the quantum ground state of the system changes in some fundamental way.* At finite temperature (see Figure 1.) we have to get closer and closer to T_c to observe the finite temperature critical behaviour. We must emphasize that in such finite temperature phase transition quantum mechanics may be important in the microscopic scale (e.g., in superconductor and superfluids quantum mechanics is needed for the existence of order) but not at the longer length scales that controls the critical behaviour and (long wavelength fluctuations are classical). The quantum

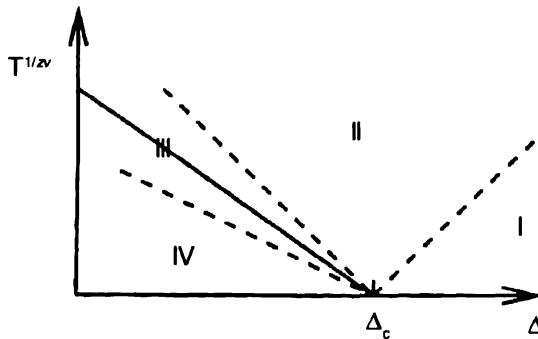


Figure 1 : A phase diagram in which the vertical axis is temperature (to the power $1/\nu$ where ν is the dynamical exponent and ν the correlation length exponent) and the horizontal axis is a parameter, Δ , which decreases T_c to zero at a critical value Δ_c . The point $T = 0, \Delta = \Delta_c$ is a quantum critical point. The full line is the phase transition from a paramagnet to a magnetically ordered phase. The dashed lines denote crossovers. The various regimes are as follows. (I) quantum paramagnet, the fluctuations are predominantly quantum, (II) "quantum critical", the physics is determined by the critical ground state at Δ_c and its thermal fluctuations, (III) classical fluctuations dominate and classical critical behaviour is observed close to the phase boundary, and (IV) magnetically ordered state with predominantly quantum fluctuations. We take the temperature to the power $1/\nu$ for the vertical axis so that the phase boundary and crossover regions are straight lines near the quantum critical point.

fluctuations become truly important for zero-temperature transition (as in quantum magnets and glass [6-9], metal-insulator transition [10] *etc.*

We shall elaborate the above discussion with the simplest example of Ising model in transverse or perpendicular magnetic field. Let us start from the transverse Ising Hamiltonian with pure ferromagnetic interaction

$$H : -J \sum_{\langle ij \rangle} S_i^z S_j^z - \Gamma \sum_i S_i^x \quad (3)$$

where S_i^z and S_i^x are Pauli spin operators on the site i satisfying the commutation relations

$$[S_i^\alpha, S_j^\beta] = 2i\epsilon_{\alpha\beta\gamma}\delta_{ij}S_i^\gamma.$$

The physical importance of the present model, from the point of view of the ferroelectric order-disorder transition in KDP systems will be discussed in the next section. We shall focus here on the quantum critical aspect of the model. In the above Hamiltonian, the presence of noncommuting term S_i^x is present which makes the Hamiltonian quantum mechanical. Here, clearly the strength of the perpendicular magnetic field Γ is to be identified with the parameter Δ of the previous discussions. One can easily check that S_i^x operating on an up-state (eigenstate with eigenvalue +1) of the operator S_i^z makes it a down state (eigenstate with eigenvalue -1). In the simplest situation, when both the thermal and quantum fluctuations are absent *i.e.* $T=0$, $\Gamma=0$, the Hamiltonian (which is simply our good old classical Ising Hamiltonian) has a complete ferromagnetically ordered ground state with all $S_i^z = +1$. Keeping Γ fixed at zero, if one increases temperature thermal fluctuations destroy ferromagnetic ordering so that $m^z (= \langle S^z \rangle)$ decreases from unity and eventually it vanishes at a particular value of temperature which is essentially the classical Ising T_c . Similarly, at $T=0$, if Γ is increased the ground state of the entire Hamiltonian is no longer completely ordered, ferromagnetic, and m^z decreases. Finally at a critical T_c , average magnetisation (over the ground state) vanishes.

Thus the phase transition in the above Hamiltonian is essentially governed by two tunable parameters T and Γ . In the presence of a small Γ , naturally transition temperature T_c from the ferromagnetic ($m^z \neq 0$) to the paramagnetic ($m^z = 0$) will be lowered. For a particular value of $\Gamma = \Gamma_c$, T_c will vanish, *i.e.*, even at $T=0$ if we increase the value of Γ eventually there will be a transition (dictated by quantum fluctuations) from ferromagnetic ($m^z \neq 0$) to the paramagnetic ($m^z = 0$) phase. The point ($T=0$, $\Gamma = \Gamma_c$) is the quantum critical point in the transverse Ising model and the above zero-temperature transition is clearly a quantum phase transition. We shall later discuss how the zero-temperature transition in the above model is related to the thermal phase transition in an equivalent classical model.

There are several other fascinating examples of quantum phase transitions in different systems which we simply mention of :

- a) The superconductor-insulator transition where the parameter Δ is the charging energy of the Josephson junction arrays.
- b) The magnetic field in quantum Hall systems controls the transition between the quantised Hall plateaus.
- c) Doping in the parent compound of a high T_c superconductor destroys the antiferromagnetic spin order.

d) Changing the amount of disorder in a conductor causes a metal-insulator transition.

In classical statistical mechanics, dynamics and its statics are separable, *i.e.*, there is no need to discuss dynamics to obtain the static critical behaviour. Stated more formally, calculating the classical partition function Z only requires the knowledge of the Hamiltonian function but not of the equation of motion. This freedom is lost in quantum problem since coordinates and momenta do not commute. It is clear that quantum phase transition is governed by the noncommutativity of the operators in the Hamiltonian and the same commutation relations govern the dynamics. *One must include dynamics at the start in describing quantum critical phenomena.* Thus time and spatial coordinates are in the same footing in quantum critical phenomena.

Essential features of quantum phase transition

We shall put down the essential features of quantum phase transition which will be more clear as we proceed with the review :

a) Quantum Phase Transition is a zero-temperature phenomena occurring in many-body interacting quantum Hamiltonians dictated by quantum fluctuations arising due to the presence of non-commuting terms in the quantum Hamiltonian.

b) Finite temperature transition in the above Hamiltonian is essentially of thermal nature due to critical slowing down.

c) Even though the QPT is a characteristic of zero-temperature which is unattainable, the quantum effects strongly dominate the crossover regions at small finite temperature. Hence, one can observe quantum effects without probing at $T = 0$ exactly.

d) In the case of pure systems the zero-temperature transition in the quantum Hamiltonian in d -dimensions is equivalent to (*i.e.*, belong to the same universality class) the thermal phase transition in an equivalent classical model in $(d + 1)$ -dimensions the additional dimension being

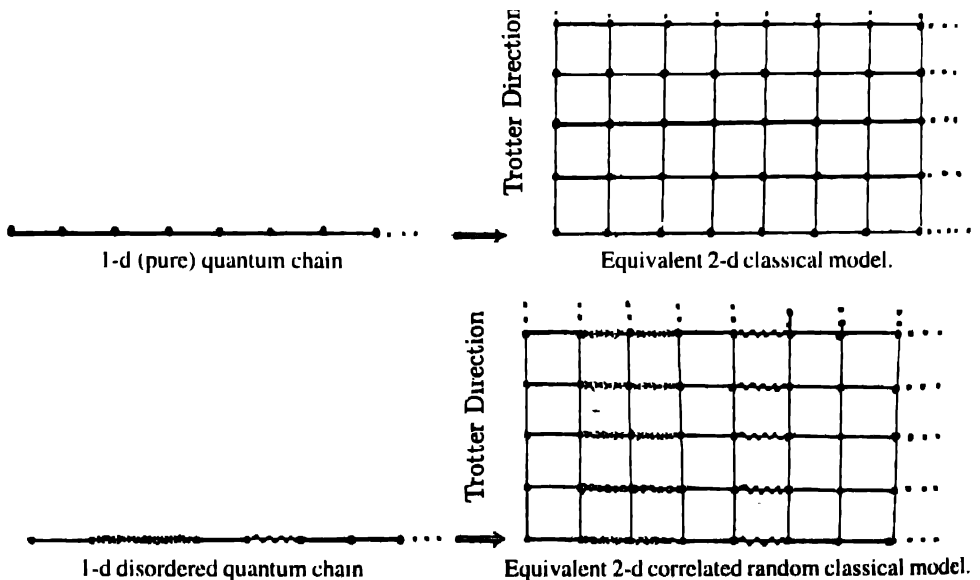


Figure 2.

the “imaginary time” direction or Trotter dimension (Figure 2). Consequently, the quantum transition is described in terms a diverging spatial correlation length ξ and a diverging time scale (correlation length in the Trotter direction) ξ_τ . In the vicinity of the quantum critical point ξ_τ grows as

$$\xi_\tau \sim \xi^z, \quad (4)$$

where z defines the dynamical exponent associated with the QPT. For pure systems $z = 1$, indicating that the space and time scale in identical fashion. It can also be shown that in the above mentioned quantum-classical mapping the ground state energy and the energy gap of the quantum Hamiltonian map to the free energy and the inverse of temporal correlation (ξ_τ) of the equivalent classical Model. In section 3, we shall elucidate the idea of quantum-classical mapping using the “Suzuki-Trotter” formalism.

e) The finite temperature transition in the quantum system are always classical is equivalent a d -dimensional classical phase transition. In the finite temperature, the quantum Hamiltonian can be mapped to a d -dimensional classical model with a finite Trotter dimension $\sim \hbar\beta$. Thus temperature delimits the width of the Trotter dimension. It will be also shown later in the “Scaling” section how the quantum effects manifest in the cross-over regions at small but finite temperature.

f) In the presence of quenched randomness, one can always employ the same machinery to map the disordered quantum Hamiltonian to an equivalent classical Hamiltonian in $(d + 1)$ -dimensions but in this case, the same pattern of randomness is repeated along the “time” direction. The disorder is found to be correlated in the time direction causing ξ and ξ_τ to diverge quite differently (*i.e.*, z is different from unity). The presence of quenched disorder modifies the phase transition in quantum systems in a very interesting fashion. We shall try to focus on those aspects in the concluding section.

2. Transverse Ising model

2.1 The model :

The study of the transverse Ising Hamiltonian dates back to the early 1960s. de Gennes [11], in 1963, studied this system to theoretically model the order-disorder transition in some double-well ferroelectric systems [12], such as potassium dihydrogen phosphate (KDP or KH_2PO_4) crystals. The mean field phase diagram [13] and the study of susceptibilities (correlations) gave good qualitative agreement with the experimental results for such simple hydrogen-bonded ferroelectric samples. It should be mentioned that Katsura [14] had already studied this model as a special case of the anisotropic Heisenberg Hamiltonian in a magnetic field and calculated the exact free energy and the dispersion relation obeyed by the elementary excitations for the one-dimensional transverse Ising system. Later, this was rederived [15] using Jordan-Wigner transformation of spins to spinless fermions and extended for the estimation of correlations. It was also studied on a chain and on a Bethe lattice [16] and its transverse susceptibility was perturbatively calculated, by employing high-temperature and low-temperature series expansions. In fact, the one-dimensional transverse Ising Hamiltonian appeared as a limit in the partition function of the two-dimensional classical Ising model on a square lattice [17]. It was soon established that the transverse Ising system is the simplest one to exhibit zero-temperature quantum phase transition (driven by quantum fluctuations arising due to the transverse field or the tunnelling term) and the zero-temperature quantum phase

transition in dimension d belongs to the same "universality" class as that of the $(d + 1)$ -dimensional classical Ising model [18-20]. In fact, the pseudo-spin mapping of the BCS Hamiltonian of superconductivity also reduces it (in the low-lying excited-state space) to an XY model in a transverse field, and in its mean field treatment it becomes exactly like that of a transverse Ising system and gives the BCS gap equation [21]. Very recently, various transverse Ising systems have been studied intensively in the context of investigations on quantum glasses (using Ising spin glass in a transverse field) [22, 23], on the nature of the quantum-fluctuation-driven ground states of antiferromagnetic or other regularly frustrated systems (using an axial next-nearest-neighbour Ising model in a transverse field) [24, 25]. These studies on the static and dynamic properties of the random (and frustrated) transverse Ising models have recently inspired intensive research on the nature of the various fluctuation-induced (and stabilised) "solid", "liquid" or "glassy" phases in quantum many-body systems. Such studies, and the progress already made with established results, imply again that the Ising model (with disorder, *etc.*) in a transverse field might be the simplest nontrivial quantum many-body system (compared to the Heisenberg system, *etc.*), having many intriguing and rich properties.

2.2 A simple version of the model and mean field phase diagram :

As mentioned earlier, de Gennes [11] introduced this model to investigate theoretically the ordered configuration of protons and elementary excitations above this ordered configuration, in the ferroelectric phase of KDP. Since each proton of the hydrogen bond of KDP can occupy one of the two minima of the double-well created by oxygen atoms [12], one can associate a double-well potential with each proton site. In the pseudo spin picture, one can ascribe a pseudo-spin $S_i^z = 1$ with the i -th proton, such that $S_i^z = 1$ corresponds to one of the well states at the site i and $S_i^z = -1$ corresponds to the other. In this pseudo-spin representation, the Hamiltonian of the proton system can be written as

$$H = -\Gamma \sum S_i^x - \sum J_{ij} S_i^z S_j^z \quad (5)$$

where S^a are the Pauli spin operators, J_{ij} is the electrostatic dipolar interaction between the (neighbouring) protons, and Γ is the tunnelling integral, which determines the rate of tunnelling of protons from one potential minima to the other [12] (S_i^x acting on the state $S_i^z = 1(-1)$ changes it to the state $S_i^z = -1(1)$). In this pseudo-spin picture, one can explain the phenomenon of ferroelectricity in the following way. In absence of any dipolar interaction between protons, the ground state of the protonic system is the symmetric combination of the states corresponding to the minima of a double well (in the pseudo-spin language the net magnetisation in the z direction vanishes ; $\langle S^z \rangle = 0$). Due to the presence of dipole-dipole interaction (J_{ij}) because of the asymmetry of the proton position, the ground state will no longer be symmetric (resulting in the ferroelectric order represented by the nonzero value of $\langle S^z \rangle$). Consequently, there will be a competition between the ordering term (J_{ij}) and delocalising or tunnelling term (Γ), arising due to the fact that the barrier separating the double-well is finite in width and height. The ordering term (J_{ij}) therefore helps the stabilisation of order (nonzero $\langle S^z \rangle$) by localising the proton in one side of the double well, and the disordering tunnelling term (Γ) competes with it and tries to delocalise the protons from any specific well. Thus, even at zero temperature, a (quantum) order-disorder transition occurs when the tunnelling term, which can

be tuned by deuteration (replacing the proton mass of hydrogen by that of deuterium) or by increasing the pressure on the sample (*i.e.*, increasing double-well overlap integral, *etc.*), is changed.

The ground state of the Hamiltonian (5) is obtained by using a semiclassical approximation, where one puts $S_i^z = S \cos \theta$ and $S_i^x = S \sin \theta$, so that the energy per site from the above Hamiltonian (5) is given by

$$E = -S\Gamma \sin \theta - S^2 J(0) \cos^2 \theta, \quad (6)$$

where $J(0) = \sum_j J_{ij}$. With the magnitude $S = 1$ here (for the two-spin state of the double well), the energy is minimised for the condition

$$\sin \theta = \Gamma / J(0), \quad (7)$$

which suggests that if $\Gamma < J(0)$, the ground state is partially polarised (both $\langle S^z \rangle$ and $\langle S^x \rangle$ are nonzero and $\langle S^z \rangle / S = 1$ and $\langle S^x \rangle = 0$ for $\Gamma = 0$), whereas for $\Gamma \geq J(0)$, the ground state is polarised in the x direction ($\langle S^x \rangle / S = 1$; $\langle S^z \rangle = 0$). Hence, as Γ increases from 0 to $J(0)$, the system undergoes a transition from a ferro-electric phase (with order parameter $\langle S^z \rangle \neq 0$) to a para-electric phase (with $\langle S^z \rangle = 0$).

In general, the finite-temperature behaviour of the above pseudo-spin model of ferroelectricity is obtained by using the mean field theory [13]. Using this approximation, one can reduce the many-body Hamiltonian (5) to a collection of effective (single) spins with Hamiltonian

$$H = - \sum_i \mathbf{h}_i \cdot \mathbf{S}_i, \quad (8)$$

where \mathbf{h}_i is the effective molecular field (Figure 3) at the site i , which is a vector in the pseudo-spin space given by $\mathbf{h}_i = \Gamma \hat{x} + \sum_j J_{ij} \langle \mathbf{S}_j \rangle$, and $\mathbf{S} = S^z \hat{z} + S^x \hat{x}$. Here, \hat{x} and \hat{z} denote respectively unit vectors in the pseudo-spin space along x and z directions.

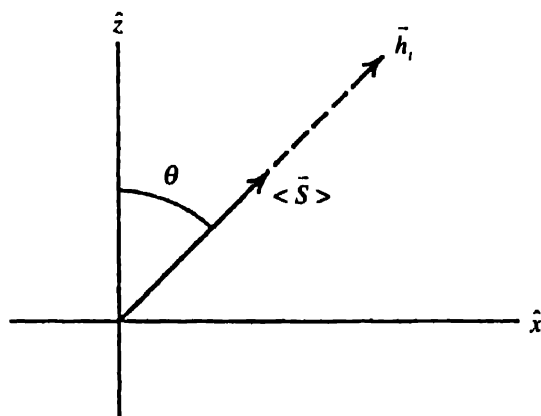


Figure 3 : The effective molecular field \mathbf{h}_i at the site i .

For the non-random case (when J_{ij} 's are not site or configuration dependent), the mean field equation for the spontaneous magnetisation can be readily written as

$$\langle S \rangle = [\tanh(\beta |h|)] |h| / |h|; \quad |h| = \sqrt{\Gamma^2 + (J(0) \langle S^z \rangle)^2}, \quad (9)$$

which gives for the components along the \hat{x} and \hat{z} directions as

$$\langle S^z \rangle = [\tanh \beta |h|] \left(\frac{J(0) \langle S^z \rangle}{|h|} \right), \quad \langle S^x \rangle = [\tanh \beta |h|] \frac{\Gamma}{|h|},$$

where $\beta = (1/k_B T)$ denotes the inverse temperature and $J(0) = \sum_j J_{ij}$. From the self-consistent solution of the above equations, one can get the mean field phase diagram (Figure 4). At $T = 0$, one gets ferroelectric order (*i.e.*, $\langle S^z \rangle \neq 0$) for $J(0) > \Gamma$, while it disappears ($\langle S^z \rangle = 0$) for $\Gamma \geq J(0)$. The transition point is given by

$$\tanh(\beta_c \Gamma) = \Gamma / J(0). \quad (10)$$

Also, as $(\tanh \beta |h|) / |h|$ is a constant ($= 1/J(0)$) for $\langle S^z \rangle \neq 0$, $\langle S^x \rangle = \text{constant}$ for $T > T_c$ and $\langle S^x \rangle = \Gamma / T$ for higher temperatures (see Figure 4).

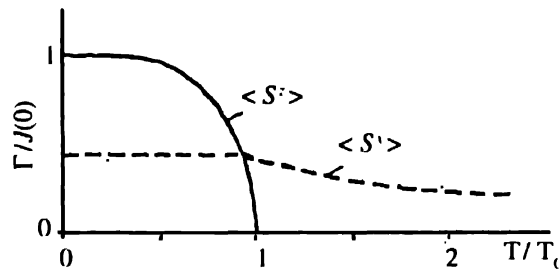


Figure 4 : Temperature dependence of $\langle S^z \rangle$ and $\langle S^x \rangle$ in the molecular field approximation

In fact, one can also study the elementary excitations of the system, considered as spin waves, using Heisenberg equation of motion obtained from Hamiltonian (1.1) (for $\hbar = 1$)

$$\ddot{S}_i^z = 2i\Gamma \dot{S}_i^x = 4\Gamma \sum_j J_{ij} S_i^x S_j^x - 4\Gamma^2 S_i^x \quad (11)$$

Using now Fourier transformation ($J(q) = \sum_j J_{ij} e^{iq \cdot R_j}$) and the random phase approximation ($S_i^x S_j^x = S_i^x \langle S_j^x \rangle + S_j^x \langle S_i^x \rangle$, with $\langle S^z \rangle = 0$ in the para-phase) [1.3], one gets

$$\omega_q^2 = 4\Gamma (\Gamma - J(q) \langle S^x \rangle), \quad (12)$$

for the elementary excitations. The largest wavelength mode ($q = 0$) softens ($\omega_0 = 0$) at the same phase boundary (given by (10)).

2.3 One dimensional chain :

The exact quantum critical point of a 1-d transverse Ising chain can be obtained using *duality symmetry* and also energy gap can be exactly obtained using the *perturbation techniques* [26]. The above methods are useful in one-dimensional model only. We shall to ref. for the discussion of the above. We shall below discuss the Fermionisation technique which allows the exact calculation of the dispersion relation of 1-d transverse Ising chain.

Eigenvalue spectrum : Fermionic representation

The above spin-1/2 transverse Ising chain Hamiltonian can be exactly diagonalised, and the entire eigenvalue spectrum and eigenfunctions can be obtained by employing Jordan-Wigner transformation of the spin operators to spinless fermions [15, 27].

For this, we consider again the Hamiltonian (5) with nearest neighbour interaction, with $J_{ij} = J$ for all i, j . Using a canonical transformation

$$S^x \rightarrow S^z, \quad S^z \rightarrow -S^x,$$

we rewrite the Hamiltonian (5) as (with $J_{ij} = J$)

$$H = - \sum S_i^z - \lambda \sum S_i^x S_{i+1}^x, \quad (13)$$

where $\lambda = J / \Gamma$.

We can now express the Hamiltonian H in terms of the raising and lowering operators S_i^+ and S_i^- at every site, where

$$S_i^+ = (1/2) [S_i^x + iS_i^y]$$

$$S_i^- = (1/2) [S_i^x - iS_i^y],$$

which satisfy a mixed set of commutation relations, *i.e.*, commute on different sites and satisfy the fermionic anticommutation relations on the same site :

$$[S_i^-, S_j^+] = 0, \quad [S_i^-, S_j^+] = 0; \quad i \neq j$$

and

$$[S_i^-, S_i^+]_+ = 1,$$

$$[S_i^-, S_i^-]_+ = [S_i^+, S_i^+]_+ = 0.$$

The last condition implies that if an arbitrary state $|F\rangle$ is not annihilated by S_i^+ , then it is annihilated by S_i^{+2} (a spin can be flipped only once) :

$$S_i^+ [S_i^+ |F\rangle] = 0; \quad S_i^{+2} = 0.$$

The above equation implies that although the operator S_i^+ creates a bosonic excitation at the site i , it is impossible to have two such excitations at the same site. This is the hard-sphere condition, and the raising and lowering operators should appropriately be treated as hard-core bosons.

The standard procedure to treat one dimensional hard-core bosons is to transform the spin operators into fermions by using the Jordan-Wigner transformation

$$c_i = \prod_{j=1}^{i-1} \exp[i\pi S_j^+ S_j^-] S_i^- \quad (14a)$$

$$c_i^\dagger = S_i^+ \prod_{j=1}^{i-1} \exp[-i\pi S_j^- S_j^+] \quad (14b)$$

One can easily check that the operators c_i and c_i^\dagger are fermionic operators satisfying

$$\{c_i, c_j^\dagger\}_+ = \delta_{ij}; \quad [c_i, c_j]_+ = 0. \quad (15)$$

Unlike the spin operators, the fermion operators anticommute even at different sites and this is due to the presence of the nonlocal factor

$$K_i = \exp \left[i\pi \sum_{j=1}^{i-1} S_j^+ S_j^- \right],$$

which is called the disorder or "soliton" term which provides an extra minus sign to convert a commutator to an anticommutator at different sites. This term is a unitary operator which rotates (upto a phase factor) the spin configuration of all sites left to the i th site by an angle π about the z -axis. This term is called the disorder term since it cannot have a nonzero expectation value in a state having a long-range order. On the other hand, it may have a nonzero expectation value in a state having no long-range order. We can therefore transform the spin system into a system of spinless fermions with chemical potential zero, defined on a one dimensional lattice

To write the Hamiltonian (13), in terms of Jordan-Wigner fermions, we need to worry about the boundary condition. If the spin chain has a periodic boundary condition, *i.e.*

$$S_1^\alpha = S_{N+1}^\alpha; \quad \alpha = x, y, z$$

then we can recast the transverse Ising Hamiltonian in the following form

$$H = N - 2 \sum_i c_i^\dagger c_i - \lambda \sum_i [c_i^\dagger - c_i][c_{i+1}^\dagger - c_{i+1}], \quad (16)$$

where we have neglected the correction term $[(c_1^\dagger + c_1)(c_N^\dagger - c_N)\{\exp(i\pi L) + 1\}]$, where $L = \sum_{i=1}^N c_i^\dagger c_i$, arising from the periodic boundary condition of spins for large systems. One must note here that although the number of fermions $\sum c_i^\dagger c_i$ is not a constant of motion, its parity is conserved and hence $\exp(i\pi L)$ is a constant of motion having the value $+1$ or -1 . Hence, the fermion problem must have an antiperiodic boundary condition if there is an even number of fermions and periodic boundary condition if there is an odd number of fermions. The correction term can be neglected for a thermodynamically large system in which case we call it the "c-cyclic" problem (the original problem being the "a-cyclic" one). Henceforth, we shall drop the constant factor N appearing in (16). One can check that it does not appear in the final diagonalised form of the transverse Ising Hamiltonian. The above transformed Hamiltonian is already quadratic in the fermion operators and it is obviously diagonalisable. To do so, let us

consider fermions in momentum space

$$c_q = (1/N)^{1/2} \sum_{j=1}^N c_j \exp[iqR_j], \quad (17)$$

$$c_q^\dagger = (1/N)^{1/2} \sum_{j=1}^N c_j^\dagger \exp[-iqR_j], \quad (18)$$

where the complete set of wavevector is $q = 2\pi m/N$,

$$m = -(N-1)/2, \dots, 0, \dots, (N-1)/2 \quad (\text{for } N \text{ even}),$$

$$m = -N/2, \dots, 0, \dots, N/2 \quad (\text{for } N \text{ odd})$$

and the final form of the transverse Ising chain Hamiltonian becomes

$$H = -2 \sum_q (1 + \bar{\lambda} \cos q) c_q^\dagger c_q - \bar{\lambda} \sum_q (e^{-iq} c_q^\dagger c_{-q}^\dagger - e^{iq} c_q c_{-q}). \quad (19)$$

To diagonalise the Hamiltonian, we employ the Bogoliubov transformation in which new fermion creation operators η_q^\dagger are formed as a linear combination of c_q^\dagger and c_q in order to remove terms in Hamiltonian which do not conserve the particle number.

For this, it is convenient to sum over modes with $q > 0$ and include the others by simply writing them out. Then above Hamiltonian (19) becomes

$$H = -2 \sum_q (1 + \bar{\lambda} \cos q) (c_q^\dagger c_q + c_{-q}^\dagger c_{-q}) + 2i\bar{\lambda} \sum_{q>0} \sin q (c_q^\dagger c_{-q}^\dagger + c_q c_{-q}). \quad (20)$$

Note that the vacuum of H is not the vacuum of the operator c_q because of the presence of the nondiagonal term $(c_q^\dagger c_{-q}^\dagger + c_q c_{-q})$ in the Hamiltonian. We wish to write the Hamiltonian in the form

$$H = \sum_q \omega_q \eta_q^\dagger \eta_q + \text{const}, \quad (21)$$

so that the single particle excitations are identifiable above the vacuum state $(\eta_q | 0) = 0$. This is achieved by making a canonical transformation from the operators c_q, c_q^\dagger to the operators η_q, η_q^\dagger (Bogoliubov transformations)

$$\eta_q = u_q c_q + i v_q c_{-q}^\dagger, \quad \eta_{-q} = u_q c_{-q} - i v_q c_q^\dagger, \quad (22)$$

$$\eta_q^\dagger = u_q c_q^\dagger - i v_q c_{-q}, \quad \eta_{-q}^\dagger = u_q c_{-q}^\dagger + i v_q c_q, \quad (23)$$

where $q > 0$ everywhere. The functions u_q, v_q are determined by two criteria: 1) these new set of operators η_q, η_q^\dagger are fermionic operators. 2) the Hamiltonian (20) is diagonalised when written in terms of these operators. The choice of the transformation is made in the way such that u_q, v_q are real. The first criterion

$$[\eta_{q'}, \eta_q^\dagger]_+ = \delta_{q',q}, \quad [\eta_{q'}, \eta_q]_+ = 0 = [\eta_q^\dagger, \eta_q^\dagger]_+,$$

leads to the relation

$$u_q^2 + v_q^2 = 1. \quad (24)$$

Using now the inverse transformation of (22,23), we can rewrite the Hamiltonian H in terms of the Bogoliubov fermions

$$\begin{aligned} H = & \sum_{q>0} [-2(1 + \bar{\lambda} \cos q)(u_q^2 + v_q^2) + 4\bar{\lambda}(\sin q)u_q v_q](\eta_q^\dagger \eta_q + \eta_{-q}^\dagger \eta_{-q}) \\ & + \sum_{q>0} [4i(1 + \bar{\lambda} \cos q)u_q v_q + 2i\bar{\lambda}(\sin q)(u_q^2 - v_q^2)](\eta_q^\dagger \eta_{-q}^\dagger + \eta_q \eta_{-q}). \end{aligned} \quad (25)$$

To recast the Hamiltonian in the diagonal form, we demand that the coefficient of the off-diagonal term must vanish

$$4(1 + \bar{\lambda} \cos q)u_q v_q + 2\bar{\lambda}(\sin q)(u_q^2 - v_q^2) = 0. \quad (26)$$

If one parametrises the coefficients u_q and v_q in the form

$$u_q = \sin \theta_q, v_q = \cos \theta_q,$$

then the condition (26) writes as

$$\tan 2\theta_q = -\frac{\bar{\lambda} \sin q}{(1 + \bar{\lambda} \cos q)}$$

Using the above condition in (25) and with some more algebra, one can write the Hamiltonian in a diagonal form

$$H = 2 \sum_q (1 + 2\bar{\lambda} \cos q + \bar{\lambda}^2)^{1/2} \eta_q^\dagger \eta_q + \text{const}, \quad (27)$$

where the constant is the zero-point energy of the spinless fermion system given by

$$E_0 = - \sum_q \omega_q. \quad (28)$$

The above equation implies that the one-dimensional transverse Ising (spin-1/2) system can be mapped into a set of noninteracting fermions, whose dispersion relation is given as

$$\omega_q = (1 + 2\bar{\lambda} \cos q + \bar{\lambda}^2)^{1/2}, \quad (29)$$

and the Bogoliubov fermion operators are written as the linear combination of the original Jordan-Wigner fermions

$$\eta_q = \sum_i \left[\left(\frac{\phi_{qi} + \psi_{qi}}{2} \right) c_i + \left(\frac{\phi_{qi} - \psi_{qi}}{2} \right) c_i^\dagger \right]. \quad (30)$$

where for $\bar{\lambda} \neq 1$ the normal modes [15] are given by

$$\psi_{qj} = \left(\frac{2}{N}\right)^{1/2} \sin(qR_j); \quad q > 0 \quad (31)$$

$$= \left(\frac{2}{N}\right)^{1/2} \cos(qR_j); \quad q \leq 0, \quad (31b)$$

$$\psi_{qj} = -\omega_q^{-1} \left[(1 + \bar{\lambda} \cos q) \phi_{qj} + \bar{\lambda} \sin q \phi_{-qj} \right]. \quad (31c)$$

For $\bar{\lambda} = 1$ and $m = -1/2$ (i.e., $q = -\pi$),

$$\omega_q = 0, \quad \phi_{qj} = N^{-1/2}, \quad \psi_{qj} = \pm N^{-1/2}. \quad (32)$$

One can thus transform the spin Hamiltonian into a noninteracting set of fermions obeying the dispersion relation given by (29).

The energy of the elementary excitations as a function of wave vector $q' = \pi - q$ for different values of $\bar{\lambda}$ is shown in the Figure 5. There is an energy gap in the excitation spectrum of the system which goes to zero at $q' = 0$ for $\bar{\lambda} \equiv \bar{\lambda}_c = 1$ as

$$\Delta(\bar{\lambda}) \equiv E_1 - E_0 = 2|1 - \bar{\lambda}|, \quad (33)$$

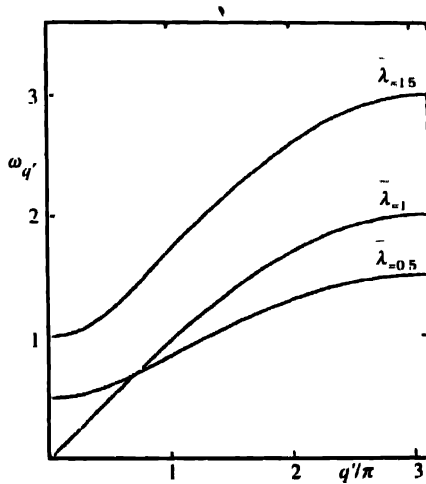


Figure 5 : Elementary excitation energy as a function of q' / π for different $\bar{\lambda}$ [2.3]

indicating the divergence of the correlation length and a quantum phase transition at $\bar{\lambda} = \bar{\lambda}_c = 1$ from an ordered state ($\langle S^x \rangle = 1$) to a disordered state ($\langle S^x \rangle = 0$). One should mention at this point that the critical value of the transverse (tunnelling) field, obtained from the exact solution of the one-dimensional chain, is $\Gamma_c = J$, whereas the mean field theory employed by Brout *et al* [13] (see Section 2.2), overestimates Γ_c for the one-dimensional nearest neighbour chain and yields $\Gamma_c = 2J$.

At this point, we remark on the simplification resulting from the consideration of the “c-cyclic” problem rather than the “a-cyclic” problem. The Hamiltonian for the “a-cyclic” problem is complicated by the presence of the term

$$[(c_1^\dagger + c_1)(c_N^\dagger - c_N)] [\exp(i\pi L) + 1].$$

As mentioned earlier, that although L is not a constant of motion, $\exp(i\pi L)$ is. Now in the ground state of the “c-cyclic” problem, in all states with even number of excitations, the number of fermions is odd (the q ’s are assumed to be occupied symmetrically around $q = 0$, except that $q = \pi$ but not $q = -\pi$ is occupied). Therefore, the additional term gives zero acting on such states and they remain eigenstates of the “a-cyclic” problem. States with odd number of excitation, on the other hand, have L even, giving an additional term in the Hamiltonian. This has the effect of making changes of the order of $1/N$ in the q ’s, ϕ_q ’s etc., which one can ignore for a thermodynamically large system. Strictly speaking the elementary excitations are not independent in the “a-cyclic” problems [27].

One must note that the above method of diagonalising a spin Hamiltonian in terms of free fermions is exact only in the case of pure transverse Ising chain in absence of any longitudinal field. One cannot generalise it to higher dimensional systems. For spin chains incorporating frustrations the resulting fermions are interacting and hence can not be diagonalised exactly. For random interaction and transverse field Ising chain, one can map the problem to free fermion problem but as both J_i ’s and Γ_i ’s are random one has to adopt numerical diagonalisation technique.

Suzuki-Trotter formalism :

In this section, we shall discuss the Suzuki-Trotter formalism, to derive the classical analogue of a quantum mechanical model and apply it to the case of pure transverse Ising model. Elliott *et al* [18] numerically established, from series studies, the equivalence of the ground state singularities of a d -dimensional transverse Ising model to those of the $(d + 1)$ -dimensional classical Ising model (see Figure 2). Later, Suzuki [20], using a generalised version of Trotter formula [20], analytically established that the ground state of a d -dimensional quantal spin system is equivalent to a certain $(d + 1)$ -dimensional classical Ising model with many-body interactions : the exponents associated with the ground state phase transition of the quantum system are the same as the exponents of thermal phase transition in the equivalent $(d + 1)$ -dimensional classical model, and for $d > 3$ the exponents of the quantum transition assume the mean field values of the exponents of the classical model. The interaction in the classical system is finite-ranged if the original quantum system has finite-range interaction.

The above equivalence can be analytically proved, as mentioned earlier, using the generalised form of Trotter formula [20], which can be written as

$$\exp [\hat{A}_1 + \hat{A}_2] = \lim_{M \rightarrow \infty} \left(\exp (\hat{A}_1 / M) \exp (\hat{A}_2 / M) \right)^M, \quad (34)$$

where \hat{A}_1 and \hat{A}_2 are quantum mechanical bounded operators not commuting with each other.

One can now employ the above mentioned formalism to the example of one dimensional Ising model in a transverse field. Let us start from the nearest-neighbour interacting Hamiltonian (with periodic boundary condition)

$$H = -J \sum_{j=1}^N S_j^z S_{j+1}^z - \Gamma \sum_{j=1}^N S_j^x ; S_{N+1} = S_1. \quad (35)$$

The partition function of the above quantum Hamiltonian can be written as

$$Z = \text{Tr} e^{-\beta H} = \text{Tr} \exp \left[\sum_{j=1}^N \left(K S_j^z S_{j+1}^z + \gamma S_j^x \right) \right] ; \beta = 1 / k_B T, \quad (36)$$

where $K = J\beta$, $\gamma = \Gamma\beta$. Using Trotter representation (34), and using the complete set of eigenvectors of the operator S_j^z , one can transform the partition function of the quantum Hamiltonian as

$$Z = \lim_{M \rightarrow \infty} A^{MN} \text{Tr} \exp \left[\sum_{j=1}^N \sum_{k=1}^M \left(\frac{K}{M} S_{j,k} S_{j+1,k} + K_M S_{j,k} S_{j,k+1} \right) \right], \quad (37)$$

where $A = [(1/2) \sinh(2\gamma/M)]^{1/2}$ and $K_M = (1/2) \ln \coth(\gamma/M)$. In deriving the eq (37), one uses the relation

$$\langle S | e^{\gamma S^z} | S' \rangle = [(1/2) \sinh 2\gamma]^{1/2} \exp[(1/2)(\ln \coth \gamma) SS'],$$

where $|S\rangle, |S'\rangle$ are eigenstates of operator S^z (see the Appendix A1). Equation (37) clearly indicates that by using the Trotter representation of exponential operators, one can transform the spin-1/2 transverse Ising chain to a classical Ising model on a $M \times N$ square lattice, with $M \rightarrow \infty$, having anisotropic coupling in the space and Trotter direction. In the limit $M \rightarrow \infty$, the strength of interaction in the Trotter direction, K_M , diverges logarithmically whereas the strength in the spatial direction, (K/M) , vanishes except when $\beta = \infty$ ($T = 0$). Hence, the correspondence between the quantum and the equivalent classical model strictly holds in the $T \rightarrow \infty$ limit.

It may be noted that the above example of equivalence of the quantum Hamiltonian (36) to an effective (classical) Hamiltonian

$$H_{\text{eff}} = - \sum_{j=1}^N \sum_{k=1}^M \left[\frac{K}{M} S_{j,k} S_{j+1,k} + K_M S_{j,k} S_{j,k+1} \right],$$

in the sense that $Z = \text{Tr} \exp(-\beta H_{\text{eff}})$ is identical to that of H , is not limited to one dimension. It is valid in general and gives for

$$H = - \sum_{ij} J_{ij} S_i^z S_j^z - \Gamma \sum_i S_i^x, \quad (38)$$

the effective Hamiltonian

$$H_{\text{eff}}(M) = - \sum_{k=1}^M \left[\frac{K}{M} \sum_{ij} S_{i,k} S_{j,k} + K_M \sum_i S_{i,k} S_{i,k+1} \right], \quad (39)$$

where $K_M = (1/2) \ln[\coth(\Gamma / M k_B T)]$. One should also mention here, that starting from the classical model one can (reversely) arrive at the equivalent (low-dimensional) quantum model as well [26] (see Appendix A2).

4. Quantum rotor model and its spherical limit

The quantum rotor model is another important model exhibiting zero-temperature quantum phase transition. The quantum rotor Hamiltonian is written as [7]

$$H_r = -\frac{1}{2} \sum_{ij} J_{ij} \mathbf{x}_i \cdot \mathbf{x}_j + \frac{1}{2I} \sum_i L_i^2, \quad \text{with } \mathbf{x}_i^2 = n, \quad (40)$$

where \mathbf{x}_i are n -component, fixed length vectors occupying the N sites of a d -dimensional hypercubic lattice and the operator $L_i^2 = (1/2) \sum_{\mu\nu} (L_i^{\mu\nu})^2$ is the invariant formed from the asymmetric rotor space angular momentum tensor $L_i^{\mu\nu} = x_i^\mu p_i^\nu - x_i^\nu p_i^\mu$. The moment of inertia term, which determines the strength of the quantum fluctuations, is denoted by I and J_{ij} 's denote the interaction among the rotors. In the zero-temperature limit, when the quantum fluctuations are absent, one gets an ordered ground state where the rotational $O(n)$ symmetry is spontaneously broken. In the opposite limit, $J_{ij} = 0$, the Hamiltonian H_r possesses non-degenerate ground state and each site is a spherically symmetric s -wave state. With the increase of the quantum fluctuation term, namely $1/I$, one eventually gets a quantum disordered (paramagnetic) ground state. The $n = 1$ limit of the above Hamiltonian corresponds to classical Ising-like spin models in the presence of a transverse field where the Hamiltonian has a Z_2 gauge symmetry [6]. Although this rotor like systems (for $n > 1$) has got very limited scope of experimental investigations but as mentioned previously the model exhibits a nontrivial zero-temperature phase transition and thereby might be helpful in the studies of other systems showing quantum phase transitions [7].

The quantum rotor partition function in the imaginary time representation, with relaxed spin constraint, can be put in the form [7, 28]

$$\mathcal{Z} = \int D\mathbf{x}_i(\tau) \exp(-\mathcal{A}), \quad (41)$$

with the effective classical action given as

$$\mathcal{A} = \int_0^\beta d\tau \left(\mathcal{L}_0(\tau) - \sum_{ij} J_{ij} \mathbf{x}_i(\tau) \cdot \mathbf{x}_j(\tau) \right), \quad (42)$$

where

$$\mathcal{L}_0 = \frac{1}{2g} \sum_i (\partial_\tau \mathbf{x}_i)^2 + r \sum_i \mathbf{x}_i^2 + u \sum_i (\mathbf{x}_i^2)^2. \quad (43)$$

Here, the mass parameter r is the measure of the strength of the quantum fluctuations which in the case of $n = 1$ is proportional to the strength of the transverse field [6]. We recast the n -component rotor action in the Fourier space, with next nearest neighbour interaction in the m of the d spatial directions as

$$\begin{aligned}
\mathcal{A} = & \frac{1}{2} \int \frac{d^d q}{(2\pi)^d} \frac{d\omega}{2\pi} \\
& \times \left[\omega^2 + r + p q_\alpha^2 + q_\beta^2 + (q_\alpha^2)^2 + c_\gamma q_\alpha^2 q_\beta^2 + c_\delta (q_\beta^2)^2 \right] x_q(i\omega) x_{-q}(-i\omega) \\
& + u \int \frac{d\omega_1}{2\pi} \dots \frac{d\omega_4}{2\pi} \int \frac{d^d q_1}{(2\pi)^d} \dots \frac{d^d q_4}{(2\pi)^d} \delta^d(q_1 + \dots + q_4) \delta(\omega_1 + \dots + \omega_4) \\
& (x_{q_1}(i\omega_1) \cdot x_{q_2}(i\omega_2)) (x_{q_3}(i\omega_3) \cdot x_{q_4}(i\omega_4)), \quad (44)
\end{aligned}$$

where $x_q(i\omega)$ are n -component Fourier space representation of \mathbf{x} and ω 's are continuous Matsubara frequencies. Here, the model is spherically symmetric in the subspace. Here, the mass parameter r is the measure of the strength of the quantum fluctuations which in the case of $n = 1$ is proportional to the strength of the transverse field [6].

Spherical limit

The classical spherical model [29] which is the $n \rightarrow \infty$ limit of the classical n -vector model [30] is an important exactly solved model for classical phase transition. Here, we indicate the solution of quantum rotor model in the spherical model. The partition function for the n -component rotor Hamiltonian can be put in the form

$$Z = \int D\mathbf{x} \exp \left[\int_0^\beta d\tau \mathcal{L}(\mathbf{x}(\tau)) \right], \quad (45)$$

with the effective classical action given by

$$\mathcal{L}(\mathbf{x}(\tau)) = -\frac{1}{2} I \sum_i |\partial_\tau \mathbf{x}_i(\tau)|^2 + \frac{1}{2} \sum_{ij} J_{ij} \mathbf{x}_i \cdot \mathbf{x}_j, \text{ with } \mathbf{x}_i^2(\tau) = n, \quad (46)$$

where $\mathbf{x}_i(\tau)$'s are classical imaginary time-dependent n -component vectors of length \sqrt{n} . If one now enforces the constraint $\mathbf{x}_i(\tau)^2 = n$, using an integral representation of the delta function

$$\delta[\mathbf{x}_i(\tau)^2 - n] = \int_{-\infty}^{\infty} \frac{d\sigma}{2\pi} \exp(-i\sigma [\mathbf{x}_i(\tau)^2 - n])$$

at each site (i) and time step (τ), the integral over the fields become Gaussian and the n -components decouple. The Gaussian action for the single component x is written as

$$\mathcal{L}_0(x(\tau), \sigma) = -\frac{1}{2} \sum_i (\partial_\tau x_i)^2 - \frac{1}{2} \sum_{i,j} D_{ij} x_i x_j + \frac{1}{\gamma} \sum_i i\sigma_i, \quad (47)$$

where $D_{ij} = i\sigma_i(\tau)\delta_{ij} - J_{ij}$. The corresponding single component free energy is given by

$$f(i\sigma) = -\ln Z_0 = -\ln \int D\mathbf{x} \exp \left[\int_0^\beta \mathcal{L}_0(\mathbf{x}; i\sigma) \right]. \quad (48)$$

The full partition function for the n -component system can be readily written as

$$Z_n = Z_0^n = \int D(\sigma) \exp[-nf(i\sigma)]. \quad (49)$$

In the $n \rightarrow \infty$ limit, the dominant contribution to full free energy of the system comes from the saddle point of $f(i\sigma)$. Hence,

$$f_{\text{sad}} = - \lim_{n \rightarrow \infty} \frac{1}{n} \ln(Z_n) = f[\lambda_i], \quad (50)$$

where the saddle point $\lambda_i = i\sigma_i$, is determined from the condition

$$\frac{\partial f(\lambda_i)}{\partial \lambda_i} = 0 \quad \text{giving} \quad \langle x_i(\tau)^2 \rangle = 1, \quad i = 1, 2, 3, \dots, N. \quad (51)$$

Here, the averaging is taken over the single component Gaussian action \mathcal{L}_0 . With the assumption that the undetermined multiplier λ_i is independent of site i , which is equivalent to considering the mean spherical approximation in the equivalent spherical model problem, the modified constraint equation can therefore be rewritten as

$$\sum_i x_i^2 = N. \quad (52)$$

We employ the Fourier representation (\mathbf{q}, ω_l) , where $\omega_l = \frac{2\pi l}{\beta}$, $l = 1, 2, 3, \dots$ are the Matsubara frequencies. In the case of regular frustration, the Matrix D_{ij} can be diagonalised with the eigenvalues $l\omega_q^2$, so that the saddle point may now be rewritten as

$$f_{\text{sad}} = -\ln \int D x_q(i\omega_l) D x_{-q}(-i\omega_l) \exp \left[-\frac{l}{2\beta} \sum_{l,q} (\omega_q^2 + \omega_l^2) x(\mathbf{q}, i\omega_l) x(-\mathbf{q}, -i\omega_l) \right]. \quad (53)$$

In the zero temperature limit ($\beta \rightarrow \infty$), the Matsubara frequencies are continuous and the summation $(1/\beta) \sum_n$ is replaced by an integral and we obtain the condition for zero temperature saddle point by summing over the continuous Matsubara frequencies given by

$$\sum \frac{1}{2l\omega_q} = 1. \quad (54)$$

For pure ferromagnetic interactions the eigenvalue ω_q of the matrix D_{ij} is written as (in the $q \rightarrow 0$ limit)

$$\omega_q^2 = \lambda - J_0 + q^2 + \dots$$

As in the classical case, the criticality occurs when $\lambda = \lambda_c = J_0$. The critical strength $l = l_c$ is obtained from (51), using the value of λ_c . Eq. (54) implies once again a $d \rightarrow d+1$ correspondence in the above model. The exponents in d -dimensional quantum spherical model without disorder are the same as the exponents of the classical spherical model in $(d+1)$ -dimensions [31].

5 Scaling relations

5.1 Zero-temperature scaling relations :

In this section, we shall discuss the scaling relations associated with the zero-temperature quantum phase transitions. We have shown in the previous section that the quantum phase

transition in pure systems lie in the same *universality* class as that of an equivalent classical Hamiltonian with one added dimension namely the Trotter (time) dimension. In the presence of quenched randomness, the disorder is correlated in the Trotter direction and has no dynamical fluctuations and thus gives rise to a completely different scenario. The scaling relations we discuss here are quite general and applicable to both Ising ($n = 1$) and rotor systems ($n \geq 2$) systems. General reference to this discussion would be [6-9].

We have mentioned earlier that the singularities associated with classical critical point arise due to of a diverging length scale namely the correlation length. The quantum phase transition is characterised by both a diverging correlation length ξ and a diverging correlation time ξ_τ (correlation length in Trotter direction). Physically speaking, it takes longer and longer time to propagate information across the correlation length as the critical point is approached. At this point, we shall once again recall the definition of the dynamical exponent z of a quantum phase transition. As mentioned previously, in the relaxational dynamics of a classical model, the relaxation time τ diverges as $\tau \sim |T - T_c|^{-\nu z}$ as $T \rightarrow T_c$ where z is the dynamical exponent of the classical model. In the quantum case ($T = 0$), both the spatial correlation and the temporal correlation length diverges as δ (which measures the deviation from the quantum critical point) in the manner,

$$\xi \sim |\delta|^{-\nu} ; \xi_\tau \sim \xi^z \text{ as } \delta \rightarrow 0$$

The above equation defines the correlation length exponent ν and the dynamical exponent z for the quantum systems. For pure systems, the dynamical exponent z is always unity so that the correlation length and the correlation (relaxation) time diverge in identical fashion but in quenched disordered systems z is different from unity indicating different scaling behaviour for the correlation length and the relaxation time. The mass gap of Hamiltonian ΔE (difference of energy between the ground state and the first excited state) vanishes as $\delta \rightarrow 0$ in the following manner

$$\Delta E \sim \xi_\tau^{-1} = \xi^{-z} \sim |\delta| \quad (55)$$

If we now consider a domain of linear dimension of the order of the correlation length ξ , the net correlation volume would be $\xi^d \xi_\tau = \xi^{d+z}$, where d is the spatial dimension of the system.

As mentioned previously, in the vicinity of the quantum phase transition, the only one characteristic length scale ξ and only one characteristic time scale ξ_τ , any observable measured at wavevector k and the frequency ω , will satisfy the scaling relation

$$O(\kappa, \omega, \delta) = \xi^{d_s} f(\kappa \xi, \omega \xi^z), \quad (56a)$$

where $\kappa \xi$ and $\omega \xi^z$ are scaled variables and d_s is the scaling dimension of the observable O . At the scale invariant critical point, the above scaling relation is no longer applicable since both ξ and ξ_τ have diverged to infinity. The only characteristic length scale would be $2\pi / \kappa$ at which the measurement is being made and only characteristic frequency $\omega \sim \kappa^z$. As a result, we find a simpler scaling relation from (56a)

$$O(\kappa, \omega, \delta = 0) = \kappa^{-d_s} \tilde{f}(\omega / \kappa^z) \quad (56b)$$

which reflects the presence of quantum fluctuations on each length and time scale.

We shall now derive the hyperscaling relation in the quantum case in the same spirit as in the classical case. The ground state energy density (the analogue of free energy density in the present case) has got a scaling form (using the correlation volume ξ^{d+z})

$$E(\kappa, \omega) \sim \xi^{-(d+z)} E(\kappa \xi, \omega \xi^z).$$

Near the criticality, the correlation length $\xi \sim \delta^{-\nu}$ and the ground state energy density $E \sim |\delta|^{2-\alpha}$, (which defines the specific heat exponent in the present case) so that we find using the scaling behaviour of the ground state energy density the hyperscaling relation given as

$$2 - \alpha = \nu(d + z).$$

If the quantum system is free from quenched disorder, the dynamical exponent $z = 1$, so the above hyperscaling relation indicate the fact that the exponents associated with quantum phase transitions in the pure system are the same as exponents are the same as equivalent classical phase transition. Clearly, the upper critical dimension of the pure quantum system is 3 in contrast to the classical case where it is 4. But in the disordered system situation is fairly complicated as emphasized previously.

We shall now study the nature of correlation function and derive the other scaling relations existing in the quantum phase transition. In the case of finite temperature transition in the vicinity of the critical point the two point correlation function satisfies the scaling form

$$G(r) \sim \frac{1}{r^{d-2+\eta_d}} f_s(r/\xi), \quad (57)$$

where as f_s is the scaling function and η_d the anomalous dimension in the classical case. At the critical point, ξ diverges yielding a purely algebraic decay of correlation function. Using eq. (54), one can now write the generic scaling form of the dynamical correlation function $G(\kappa, \omega)$ given as

$$G(\kappa, \omega) = \langle S_{\kappa}(i\omega) S_{-\kappa}(-i\omega) \rangle \sim \xi^{2-\eta} f(\kappa \xi, \omega \xi^z), \text{ as } \kappa, \omega \rightarrow 0, \quad (58)$$

where $2 - \eta$ is the scaling dimension of the observable $G(\kappa, \omega)$ and η is the anomalous dimension for the dynamic correlation function in quantum phase transition. At the quantum critical point, we have similarly the simpler scaling form given as

$$G(\kappa, \omega) = \langle S_{\kappa}(i\omega) S_{-\kappa}(-i\omega) \rangle \sim \kappa^{-(2-\eta)} \bar{f}(\omega/\kappa^z), \text{ as } \kappa, \omega \rightarrow 0. \quad (59)$$

The fluctuation-dissipation theorem [32] gives us the following relation between wave-vector dependent static susceptibility $\chi(\kappa)$ and the dynamic k -dependent correlation function $G(\kappa, \omega)$ at $T = 0$.

$$\chi(\kappa) = \int \frac{d\omega}{2\pi} \frac{G(\kappa, \omega)}{\omega}. \quad (60)$$

The susceptibility exponent γ for the quantum transition is defined through the relation

$$\chi(\kappa = 0) \sim |\delta|^{-\gamma} \sim \xi^{\gamma/\nu}. \quad (61)$$

Using the scaling form $G(\kappa, \omega)$ in (60), we find the scaling relation connecting the exponents γ and ν of the form (using (61))

$$\gamma = (2 - \eta) \nu. \quad (62)$$

This scaling relation is identical to the scaling relation in the classical case because it does not depend upon the dimensionality of the system.

We conclude the above section on scaling with following comments :

a) The finite temporal correlation means a gap in the spectrum of the quantum problem. The quantum critical point is *gapless*. Often, in quantum Ising systems with disorder, either side of the QCP is flanked by regions where ξ_τ diverges (see Section 6).

b) The exponent z is the characteristic of the critical point and has nothing to do with the either phases.

c) As in the case of classical phase transition, in this case also there is a wide range of *universality*.

5.2 Finite-temperature scaling :

The effect of finite temperature is essentially to reduce the effective dimensionality of the problem. At $T \neq 0$, the Trotter dimension is finite (or in other words, the Matsubara frequencies are discrete) and the equivalent classical system now resemble a hyperslab of d -spatial dimensions and one temporal dimension of size $L_\tau = \hbar\beta$. As mentioned previously, the dimensionality of the system is going to determine the relative strength of the critical fluctuations and that is why the finite size in the Trotter direction is going to affect the critical behaviour in a non-trivial fashion. The finiteness of L_τ causes a crossover away from the $T=0$ critical point, it does so in a fashion controlled by the physics at that critical point. When the coupling K is far away from the quantum critical coupling K_c , both the correlations ξ and ξ_τ are small and hence the system is effectively $d+1$ -dimensional. As K approaches K_c , ξ and consequently ξ_τ increases and as ξ_τ exceeds L_τ , the system "senses" the finiteness of Trotter dimension and behaves as d -dimensional classical system. The finite temperature transition in the above models are always *classical*, as we have already discussed in the introductory sections comparing the corresponding energy scales associated with the quantum fluctuations and thermal fluctuations (Fig. 1).

To extend the scaling relations to small finite temperature in the vicinity of the quantum critical point, one has to extend the idea of finite size scaling¹ to the present case.¹ Let us consider, some quantity X , which diverges at $T=0$ line as $|\delta|^{-\nu}$, the finite temperature scaling ansatz in terms of dimensionless quantities will be given as

$$X(\delta, T, \omega) = |\delta|^{-\nu} F_{\pm} \left(\frac{|\delta|^{z\nu}}{\kappa_B T}, \frac{\hbar\omega}{\kappa_B T} \right). \quad (63)$$

There are different scaling functions F_{\pm} , depending on the sign of δ . A number of important conclusions can be drawn from the above scaling ansatz. There is a singularity in the zero-frequency scaling function corresponding to the critical line, from eqn. this must occur when $k_B T / |\delta|^{z\nu}$ has a fixed value, i.e.,

$$T_c \sim |\delta|^{z\nu}. \quad (64)$$

¹ For finite size scaling see : M. E. Fisher and M. N. Barber, *Phys. Rev. Lett.* **28** 1516 (1972).

For different crossover regions we refer to the fig. 1. Cross-over from the region I to the region II occurs when

$$\kappa_B T \sim \hbar \omega_c, \quad (65)$$

since the gap ω_c scales $|\delta|^{2\nu}$, the crossover occurs when

$$T \sim \delta^{2\nu}. \quad (66)$$

The region within the dotted wedge in the vicinity of the critical curve is dominated by classical fluctuations due to *critical slowing down*.

6. Quantum phase transition in disordered systems

Following the discovery of zero-temperature transition in the dipolar Ising transverse field $\text{LiHo}_1Y_{1-x}F_4$ [22], there has been a recent upsurge in the study of quantum phase transitions in system in the presence of quenched randomness. These systems along with the *proton glasses* (mixture of ferroelectric and antiferroelectric materials) provide very useful experimental realisation of quantum spin glass system. In this section we shall provide a bird's eye view to this rapidly advancing subject quantum phase transition in quenched disordered systems.²

We shall start with the typical Hamiltonian which enables us to describe such quantum transition in random systems :

Quantum Spin Glass :

Ising

$$H = - \sum_{ij} J_{ij} S_i^z S_j^z - \gamma \sum_i S_i^x. \quad (67)$$

Rotor

$$H_r = - \frac{1}{2} \sum_{ij} J_{ij} \mathbf{x}_i \cdot \mathbf{x}_j + \frac{1}{2In} \sum_i L_i^2, \quad \text{with } \mathbf{x}_i^2 = n, \quad (68)$$

where the interactions J_{ij} are random with binary or Gaussian probability distribution.

Quantum Random Field Systems

Ising

$$H = - \sum_{ij} J_{ij} S_i^z S_j^z - \gamma \sum_i S_i^x - \sum_i h_i S_i^z. \quad (69)$$

Rotor

$$H_r = - \frac{1}{2} \sum_{ij} J_{ij} \mathbf{x}_i \cdot \mathbf{x}_j + \frac{1}{2In} \sum_i L_i^2 + \sum_i \tilde{h}_i \cdot \mathbf{x}_i, \quad \text{with } \mathbf{x}_i^2 = n. \quad (70)$$

In this case, the field h_i is random with binary or Gaussian probability distribution.

² For classical spin glass system see, K. Binder and A. P. Young, *Rev. Mod. Phys.* **58** 810 (1986). For classical random field systems see T. Nattermann, Cond-mat/9705295 and references therein ; *Spin Glasses and Random Fields*, ed A. P. Young, (Singapore : World Scientific) (1998).

We shall now briefly discuss how the presence of disorder nontrivially modifies the transition in above systems and what are the novel phenomena arising because of disorder. If one applies a *Suzuki-Trotter* method to obtain the classical counterpart of the above quantum disordered systems, it is readily observed that the equivalent classical system has *correlated randomness* that is randomness is correlated in the Trotter direction with interactions along the Trotter direction always being *ferromagnetic*. The scenario is clearly depicted in the Figure 2 above where we show how the randomness is correlated in the Trotter direction of the equivalent 2-dimensional model if we start from a disordered quantum chain. We find that the same pattern of randomness is being replicated along each time slice. This correlated randomness demands that *quantum transition in random systems in d -dimensions is not equivalent to a classical transition in $d+1$ -dimensions*. The spatial and temporal correlation length diverge quite differently or in other words the dynamical exponent z , is different from unity. The entirely anisotropic scaling of space and time is an artifact of the correlated randomness.

In the sense of renormalisation group, it is often found that in the presence of disorder, *the quantum fluctuation are dangerously irrelevant*. Without going into technical details of this dangerous irrelevance, we shall just mention that if some parameter say u of the Hamiltonian, vanishes as the system approaches the critical point but at the same time it causes the scaling function to diverge, the parameter is said to be *dangerously irrelevant* and shows up its effect in the hyperscaling relation. We shall refer to the [7] and [33] for the discussion on this particular aspect of quantum phase transitions.

We shall also mention here, due to the presence of *correlated randomness* the ϵ -expansion is not much useful in the study of these systems. It is found that under the *renormalisation group transformation* disorder grows and eventually one finds a "run-away" to the strong couplings and the perturbative calculations fail. It is worth mentioning that the most useful methods of studying the above have been so far *quantum Monte Carlo* methods via mapping the problem to equivalent correlated random classical system and *real space renormalisation group* calculation in low dimensions.

We shall now just briefly mention the other aspects of QPT in presence of disorder. The physics here is markedly different from the physics of classical random systems. The dynamical exponent $z (\neq 1)$ appears in the scaling relations in a nontrivial manner. Similarly, the *real time dynamics* is also quite novel, and we believe that the nature of dynamical scaling (*activated or conventional*) depends on the symmetry of the order parameter field (Ising or rotor).

The most important findings of the zero-temperature phase transition is the *Griffiths-McCoy singularity* [34]. By this, we mean that at $T = 0$ phase transition in random quantum Ising systems, there are pronounced singularities on the either side of the quantum critical point which we call Griffiths-McCoy singularities. These singularities arise due to the occurrence of *rare regions* which have stronger interaction than the average. These singularities cause susceptibility to diverge even when the system is away from the quantum critical point. The effect of these type of singularities is weaker in the case of classical disordered systems. Recently, there have been numerous theoretical studies towards understanding this Griffiths-McCoy region. Singularities arise due to regions which are *locally ferromagnetic* and thus have very small energy gap ΔE (between the ground state and the first excited state of that region, which are degenerate as the linear dimension of the region goes to infinity). Consequently, there are low energy cluster excitations, which have a power law distribution of energy ΔE . This power-law distribution signals the divergence of the correlation length ξ_c and thus the

response (linear or nonlinear susceptibility) diverges even when the system is away from criticality. These "divergence" is much feeble in the case of rotors where one does not observe a power law distribution of ΔE . The quantum critical point in the Ising case is thus flanked by regions with prominent Griffiths singular region and the dynamical exponent z varying continuously in these regions. We refer to [9, 35, 36] for a detailed discussion on the above point.

Question of replica symmetry breaking in zero-temperature transition is also being emphatically highlighted in recent studies. The debate is far from being settled till date [6, 37]

The long-range (Sherrington-Kirkpatrick) version of the quantum spin glass has been investigated extensively in recent years using both analytical and quantum Monte Carlo techniques [37, 38]. The phase diagram is obtained and also the question of replica symmetry breaking has been addresses [37].

Recently, the short range (Edwards-Anderson) model has been studied using the quantum Monte Carlo methods and the phase diagram and zero-temperature scaling relations are obtained [23].

The study of quantum random field systems are quite recent. Both the long-range interacting and short-range interacting models have been studied. The renormalisation group calculation shows the dangerous irrelevance of quantum fluctuations and the various scaling relations associated with the zero-temperature transitions. The dynamical scaling is found to be *activated* for Ising systems where it is conventional for the rotor systems [33, 39, 40].

Appendix

A1 Effective classical Hamiltonian of the transverse Ising model

To evaluate the effective classical Hamiltonian, let us start from the quantum Hamiltonian describing a transverse Ising model on a d -dimensional lattice

$$H = H_0 + V = -\Gamma \sum_i S_i^x - \sum_{ij} J_{ij} S_i^z S_j^z, \quad (\text{A1})$$

where S_j^α 's are the Pauli spin operators, as mentioned earlier. The partition function of this quantum Hamiltonian can be written as

$$Z = \text{Tr} \exp [-\beta(H_0 + V)]. \quad (\text{A2})$$

Using the generalised Trotter formula (cf. Section 3.1), one can rewrite the exponential operator in the equation (A2) as

$$\exp [-\beta(H_0 + V)] = \lim_{M \rightarrow \infty} \left[\exp \left(\frac{-\beta H_0}{M} \right) \exp \left(\frac{\beta V}{M} \right) \right]^M, \quad (\text{A3})$$

which is equivalent to considering M identical replicas of the original system. The partition function of the quantum system can readily be written (inserting set of identity operators) in the form

$$Z = \lim_{M \rightarrow \infty} \text{Tr} \prod_{k=1}^M \langle S_{1,k}, S_{2,k}, \dots, S_{N,k} \rangle$$

$$\left[\exp\left(\frac{-\beta H_0}{M}\right) \exp\left(\frac{\beta V}{M}\right) \right] |S_{1,k+1}, S_{2,k+1}, \dots, S_{N,k+1}\rangle, \quad (\text{A4})$$

where $|S_{i,k}\rangle$'s are the eigenstates of the operators S^z . It is quite clear that by inserting the sets of identity operators, one has effectively introduced an additional dimension in the problem ("Trotter dimension"), which is denoted by the index k . One then uses the following relations

$$\begin{aligned} & \prod_{k=1}^M \langle S_{1,k}, \dots, S_{N,k} | \exp\left(\frac{\beta}{M} \sum_{ij} J_{ij} S_i^z S_j^z\right) | S_{1,k+1}, \dots, S_{N,k+1} \rangle \\ &= \exp \left[\sum_{i,j=1}^N \sum_{k=1}^M \frac{\beta J_{ij}}{M} S_{i,k} S_{j,k} \right]. \end{aligned} \quad (\text{A5a})$$

$$\begin{aligned} & \prod_{k=1}^M \langle S_{1,k}, \dots, S_{N,k} | \exp\left(\frac{\beta \Gamma}{M} \sum_i S_i^x\right) | S_{1,k+1}, \dots, S_{N,k+1} \rangle \\ &= \left(\frac{1}{2} \sinh\left(\frac{2\beta \Gamma}{M}\right) \right)^{NM} \exp \left[\frac{1}{2} \ln \coth\left(\frac{\beta \Gamma}{M}\right) \sum_{i=1}^N \sum_{k=1}^M S_{i,k} S_{i,k+1} \right]. \end{aligned} \quad (\text{A5b})$$

In deriving the relation (A5b), one has to use the relation

$$\langle S | e^{aS'} | S' \rangle = [(1/2) \sinh(2a)]^{\frac{1}{2}} \exp[SS'/2 \ln \coth(a)], \quad (\text{A6a})$$

(where $|S\rangle$ and $|S'\rangle$ are the eigenstates of S^z), which can be easily derived writing the exponential operator in the form

$$e^{aS'} = \cosh(a) + S^x \sinh(a), \quad (\text{A6b})$$

which can be checked by expanding the exponential function and using $(S^x)^2 = 1$. One can now compare (A6b) with (A3), putting explicitly the eigenvalues S and S' . Using the relations (A5a,b), one can arrive at the final form of the partition function of the quantum system, with the M -th Trotter approximation

$$Z = C^{\frac{NM}{2}} \text{Tr}_v \exp(-\beta H_{\text{eff}}(S)); \quad C = \frac{1}{2} \sinh\left(\frac{2\beta \Gamma}{M}\right), \quad (\text{A7a})$$

where

$$H_{\text{eff}}(S) = \sum_{i,j=1}^N \sum_{k=1}^M \left[-\frac{J_{ij}}{M} S_{i,k} S_{j,k} - \frac{\delta_{ij}}{2\beta} \ln \coth\left(\frac{\beta \Gamma}{M}\right) S_{i,k} S_{i,k+1} \right]. \quad (\text{A7b})$$

Since $S_{i,k}$ are classical numbers (± 1), the above Hamiltonian represents a classical Ising Hamiltonian on a $(d+1)$ -dimensional lattice, with anisotropic coupling in the spatial and Trotter dimension. One must note here that for the equivalence between the quantum and

classical Hamiltonians to hold, one must consider $M \rightarrow \infty$ limit. As mentioned earlier, for infinitely large M , one must also consider the $\beta \rightarrow \infty$ limit, so that the zero-temperature phase transition in the d -dimensional quantum model is equivalent to the thermal phase transition in $(d+1)$ -dimensional equivalent classical model.

A2 Derivation of the equivalent quantum Hamiltonian of a classical spin system

Starting from a classical spin Hamiltonian, one can also (conversely) derive the equivalent quantum Hamiltonian in an extreme anisotropic limit [26]. If one considers a classical spin Hamiltonian on a d -dimensional lattice and \hat{T} denotes the transfer matrix of the classical system, the equivalent quantum Hamiltonian is defined as

$$\hat{T} = 1 - \tau H + O(\tau^2), \quad (\text{A8})$$

where τ is a strictly infinitesimal parameter (may be considered as the lattice parameter in one particular (time) direction). The Hamiltonian H corresponds to the equivalent quantum Hamiltonian of the classical system. The free energy of the statistical mechanical system, given by the largest eigenvalue of the transfer matrix, is now related to the ground state energy of the quantum Hamiltonian and the correlation length is given by the inverse of energy gap of the quantum Hamiltonian.

We shall illustrate the above mentioned equivalence using the example of a two dimensional spin-1/2 classical Ising system on a square lattice, with anisotropic coupling strengths J_1 and J_2 . The row to row transfer matrix of the above Hamiltonian can be written as (17)

$$\hat{T} = \hat{T}_1 \hat{T}_2 \hat{T}_1, \quad (\text{A9})$$

where

$$\hat{T}_1 = \exp \left[\sum_i \tilde{K}_1 S_i^x \right], \quad (\text{A10a})$$

$$\hat{T}_2 = \exp \left[\sum_i K_2 S_i^z S_{i+1}^z \right], \quad (\text{A10b})$$

with $K_i = \beta J_i$, $i = 1, 2$ and \tilde{K}_1 is given by

$$\tilde{K}_1 = -\frac{1}{2} \ln (\tanh K_1). \quad (\text{A10c})$$

Clearly the operators \hat{T}_1 and \hat{T}_2 do not commute. To write the above transfer matrix (A9) in the form (A8) one has to suitably define the expansion parameter τ . One sets [3,23] $\tau = \tilde{K}_1$, and $K_2 = \lambda \tau$, where λ is finite. One can now neglect the noncommutivity of the operators \hat{T}_1 and \hat{T}_2 if one considers the extreme anisotropic limit given by

$$K_1 \rightarrow \infty (\tilde{K}_1 \rightarrow 0) \text{ and } K_2 \rightarrow 0 \text{ with } \lambda = \frac{K_2}{\tilde{K}_1} \equiv O(1), \quad (\text{A11})$$

the transfer matrix is readily written in the form (A8) as $\tau = 0$, where the equivalent quantum Hamiltonian H is given by

$$H = - \sum_i S_i^x - \lambda \sum_i S_i^z S_{i+1}^z, \quad (\text{A12})$$

with λ playing the role of inverse temperature. One thus obtains the transverse Ising Hamiltonian from the classical Ising Hamiltonian in the extreme anisotropic limit. One should note here that this equivalence is established in the extreme anisotropic limit, $\tau, K_2 \rightarrow 0$, called the "Hamiltonian" limit. The essential assumption behind this mapping is that this anisotropy does not affect the universality class of the problem.

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